

# Investigation of continuous-time quantum walks via spectral analysis and Laplace transform

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**Abstract**

Continuous-time quantum walk (CTQW) on a given graph is investigated by using the techniques of the spectral analysis and inverse Laplace transform of the Stieltjes function (Stieltjes transform of the spectral distribution) associated with the graph. It is shown that, the probability amplitude of observing the CTQW at a given site at time  $t$  is related to the inverse Laplace transformation of the Stieltjes function, namely, one can calculate the probability amplitudes only by taking the inverse laplace transform of the function  $iG_\mu(is)$ , where  $G_\mu(x)$  is the Stieltjes function of the graph. The preference of this procedure is that, there is no any need to know the spectrum of the graph.

**Keywords:**Continuous-time quantum walk, QD and non-QD type graphs, Stieltjes function, Laplace transformation

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# 1 Introduction

One of the most challenging problems in quantum computation has been the design of quantum algorithms which outperform their classical counterparts in meaningful tasks. Few quantum codes in this category have been discovered after the well-known examples by Shor and Grover [1, 2]. A natural way to discover new quantum algorithmic ideas is to adapt a classical one to the quantum model. An appealing well-studied classical idea in statistics and computer science is the method of random walks [3, 4]. Recently, the quantum analogue of classical random walks has been studied in a flurry of works [5, 6, 7, 8, 9, 10]. The works of Moore and Russell [9] and Kempe [10] showed faster bounds on instantaneous mixing and hitting times for discrete and continuous quantum walks on the hypercube (compared to the classical walk). The focus of this paper is on the continuous-time quantum walk that was introduced by Farhi and Gutmann [5]. In Refs. [11, 12, 13], the dynamical properties of CTQW on finite and infinite graphs have been studied by using the spectral analysis. In fact, it has been shown that the probability amplitudes of the CTQW on a given graph are related to the Stieltjes function or Stieltjes transformation of the spectral distribution associated with the adjacency matrix of the graph, i.e., in order to calculate the probability amplitudes one needs to evaluate the inverse Stieltjes transformation. The Stieltjes function has extensive applications for example in solid state physics and condensed matter, where it is known as Green function. It can be also used for calculating the two-point resistances on regular resistor networks [14]. Although, with any arbitrary graph one can associate a Stieltjes function (see Ref.[15]), calculation of the inverse Stieltjes transformation is not an easy task. In this work, we show that the probability amplitudes of CTQW on graphs can be evaluated by taking the inverse Laplace transformation of the Stieltjes function which is easier and more popular transformation with respect to the inverse Stieltjes transformation. In fact, the Laplace transformation is used extensively in various problems of pure and applied mathematics. Particularly widespread

and effective is its application to problems arising in the theory of operational calculus and in its applications, embracing the most diverse branches of science and technology. An important advantage of methods using the Laplace transformation lies in the possibility of compiling tables of direct and inverse Laplace transforms of various elementary and special functions commonly encountered in applications. We survey and re-derive equations for the CTQW on QD [12, 16] and non-QD [15] type graphs by using the Laplace transformation.

The organization of the paper is as follows: In section 2, some preliminary facts about graphs and their stratifications, the quantum decomposition for the adjacency matrix of some particular graphs called QD graphs and Stieltjes transform of spectral measure associated with the graph are reviewed. In section 3, we review CTQW on an arbitrary graph and give a procedure for calculating the probability amplitudes of CTQWs on graphs by using the inverse Laplace transformation. Section 4 is devoted to some examples of CTQW on QD and non-QD type graphs and calculation of the corresponding probability amplitudes of the walk on them by employing the techniques introduced in the section 3. The paper is ended with a brief conclusion and an appendix containing a table of examples of CTQW on some important distance-regular graphs.

## 2 Preliminaries

In this section we review some preliminary facts about graphs and their stratifications, the quantum decomposition for the adjacency matrix of some particular graphs called QD graphs and Stieltjes transform of spectral measure associated with the graph.

### 2.1 Graphs and their stratifications

A graph is a pair  $G = (V, E)$ , where  $V$  is a non-empty set and  $E$  is a subset of  $\{(i, j); i, j \in V, i \neq j\}$ . Elements of  $V$  and of  $E$  are called vertices and edges, respectively. Two vertices

$i, j \in V$  are called adjacent if  $(i, j) \in E$ , and in that case we write  $i \sim j$ . A finite sequence  $i_0; i_1; \dots; i_n \in V$  is called a walk of length  $n$  (or of  $n$  steps) if  $i_{k-1} \sim i_k$  for all  $k = 1, 2, \dots, n$ . A graph is called connected if any pair of distinct vertices is connected by a walk. The degree or valency of a vertex  $x \in V$  is defined by  $\kappa(x) = |\{y \in V : y \sim x\}|$ . The graph structure is fully represented by the adjacency matrix  $A$  defined by

$$(A)_{i,j} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise} \end{cases} \quad (i, j \in V). \quad (2-1)$$

Obviously, (i)  $A$  is symmetric; (ii) an element of  $A$  takes a value in  $\{0, 1\}$ ; (iii) a diagonal element of  $A$  vanishes. Let  $l_2(V)$  denote the Hilbert space of square-summable functions on  $V$ , and  $\{|i\rangle; i \in V\}$  becomes a complete orthonormal basis of  $l_2(V)$ . The adjacency matrix is considered as an operator acting in  $l_2(V)$  in such a way that

$$A|i\rangle = \sum_{j \sim i} |j\rangle, \quad i \in V. \quad (2-2)$$

For  $i \neq j$  let  $\partial(i, j)$  be the length of the shortest walk connecting  $i$  and  $j$ . By definition  $\partial(i, j) = 0$  for all  $i \in V$ . The graph becomes a metric space with the distance function  $\partial$ . Note that  $\partial(i, j) = 1$  if and only if  $i \sim j$ . We fix a point  $o \in V$  as an origin of the graph. Then, a natural stratification for the graph is introduced as:

$$V = \bigcup_{i=0}^{\infty} V_i(o), \quad V_i(o) := \{j \in V : \partial(o, j) = i\}. \quad (2-3)$$

If  $V_k(o) = \emptyset$  happens for some  $k \geq 1$ , then  $V_l(o) = \emptyset$  for all  $l \geq k$ . With each stratum  $V_i$ , we associate a unit vector in  $l_2(V)$  defined by

$$|\phi_i\rangle = \frac{1}{\sqrt{\kappa_i}} \sum_{k \in V_i(o)} |k\rangle. \quad (2-4)$$

where,  $\kappa_i := |V_i(o)|$  and  $|k\rangle$  denotes the eigenket of  $k$ -th vertex at the stratum  $i$ . The closed subspace of  $l_2(V)$  spanned by  $\{|\phi_i\rangle\}$  is denoted by  $\Gamma(G)$ . Since  $\{|\phi_i\rangle\}$  becomes a complete orthonormal basis of  $\Gamma(G)$ , we often write

$$\Gamma(G) = \sum_k \oplus C|\phi_k\rangle. \quad (2-5)$$

In this stratification for any connected graph  $G$ , we have

$$V_1(\beta) \subseteq V_{i-1}(\alpha) \cup V_i(\alpha) \cup V_{i+1}(\alpha), \quad (2-6)$$

for each  $\beta \in V_i(\alpha)$ . Now, recall that the  $i$ -th adjacency matrix of a graph  $G = (V, E)$  is defined as

$$(A_i)_{\alpha, \beta} = \begin{cases} 1 & \text{if } \partial(\alpha, \beta) = i, \\ 0 & \text{otherwise} \end{cases} \quad (\alpha, \beta \in V). \quad (2-7)$$

Then, for reference state  $|\phi_0\rangle$  ( $|\phi_0\rangle = |o\rangle$ , with  $o \in V$  as reference vertex), we have

$$A_i|\phi_0\rangle = \sum_{\beta \in V_i(o)} |\beta\rangle. \quad (2-8)$$

Then by using (2-4) and (2-8), we have

$$A_i|\phi_0\rangle = \sqrt{\kappa_i}|\phi_i\rangle. \quad (2-9)$$

## 2.2 QD type graphs

Let  $A$  be the adjacency matrix of a graph  $G = (V, E)$ . According to the stratification (2-3), we define three matrices  $A_+$ ,  $A_-$  and  $A_0$  as follows: for  $i \in V_k$  we set

$$A_+|i\rangle = \sum_{j \in V_{k+1}} |j\rangle, \quad A_-|i\rangle = \sum_{j \in V_{k-1}} |j\rangle, \quad A_0|i\rangle = \sum_{j \in V_k} |j\rangle. \quad (2-10)$$

for  $j \sim i$ . Since  $i \in V_k$  and  $i \sim j$ , then  $j \in V_{k-1} \cup V_k \cup V_{k+1}$ , where we tacitly understand that  $V_{-1} = \emptyset$ . One can easily verify that

$$(A_+)^* = A_-, \quad (A_0)^* = A_0, \quad \text{and}$$

$$A = A_+ + A_- + A_0 \quad (2-11)$$

This is called quantum decomposition of  $A$  associated with the stratification (2-3). The vector state corresponding to  $|o\rangle = |\phi_0\rangle$ , with  $o \in V$  as the fixed origin, is analogous to the vacuum state in Fock space. According to Ref.[16], the  $\langle A^m \rangle$  coincides with the number of  $m$ -step

walks starting and terminating at  $o$ , also, by lemma 2.2 of [16], if  $\Gamma(G)$  is invariant under the quantum components  $A_+$ ,  $A_-$  and  $A_0$ , then there exist two sequences  $\{\omega_k\}_{k=1}^\infty$  and  $\{\alpha_k\}_{k=1}^\infty$  derived from  $A$ , such that

$$\begin{aligned} A_+|\phi_k\rangle &= \sqrt{\omega_{k+1}}|\phi_{k+1}\rangle, \quad k \geq 0, \\ A_-|\phi_k\rangle &= \sqrt{\omega_k}|\phi_{k-1}\rangle, \quad k \geq 1, \\ A_0|\phi_k\rangle &= \alpha_{k+1}|\phi_k\rangle, \quad k \geq 0 \end{aligned} \tag{2-12}$$

(for more details see [11, 16]). Following Ref.[11], we will refer to the graphs with this property as QD type graphs and the parameters  $\omega_k$  and  $\alpha_k$  will be called QD parameters of the graph. We note that in QD type graphs, the stratification is independent of the choice of reference state.

### 2.3 Stieltjes transform of spectral measure associated with the graph

It is well known that, for any pair  $(A, |\phi_0\rangle)$  of a matrix  $A$  and a vector  $|\phi_0\rangle$ , it can be assigned a measure  $\mu$  as follows

$$\mu(x) = \langle \phi_0 | E(x) | \phi_0 \rangle, \tag{2-13}$$

where  $E(x) = \sum_i |u_i\rangle \langle u_i|$  is the operator of projection onto the eigenspace of  $A$  corresponding to eigenvalue  $x$ , i.e.,

$$A = \int x E(x) dx. \tag{2-14}$$

It is easy to see that, for any polynomial  $P(A)$  we have

$$P(A) = \int P(x) E(x) dx, \tag{2-15}$$

where for discrete spectrum the above integrals are replaced by summation. Therefore, using the relations (2-13) and (2-15), the expectation value of powers of adjacency matrix  $A$  over starting site  $|\phi_0\rangle$  can be written as

$$\langle \phi_0 | A^m | \phi_0 \rangle = \int_R x^m \mu(dx), \quad m = 0, 1, 2, \dots \tag{2-16}$$

The existence of a spectral distribution satisfying (2-16) is a consequence of Hamburgers theorem, see e.g., Shohat and Tamarkin [[17], Theorem 1.2].

Obviously relation (2-16) implies an isomorphism from the Hilbert space of the stratification onto the closed linear span of the orthogonal polynomials with respect to the measure  $\mu$ . From (4-43) and (2-9), we have for distance-regular graphs

$$|\phi_i\rangle = P'_i(A)|\phi_0\rangle, \quad (2-17)$$

where,  $P'_i = \frac{1}{\sqrt{\kappa_i}}P_i$  is a polynomial with real coefficients and degree  $i$ . Now, substituting (2-17) in (4-44), we get the following three term recursion relations for the polynomials  $P'_j(x)$

$$xP'_k(x) = \beta_{k+1}P'_{k+1}(x) + \alpha_k P'_k(x) + \beta_k P'_{k-1}(x) \quad (2-18)$$

for  $k = 0, \dots, d-1$ , with  $P'_0(x) = 1$ . Multiplying (2-18) by  $\beta_1 \dots \beta_k$ , we obtain

$$\beta_1 \dots \beta_k x P'_k(x) = \beta_1 \dots \beta_{k+1} P'_{k+1}(x) + \alpha_k \beta_1 \dots \beta_k P'_k(x) + \beta_k^2 \beta_1 \dots \beta_{k-1} P'_{k-1}(x). \quad (2-19)$$

By rescaling  $P'_k$  as  $Q_k = \beta_1 \dots \beta_k P'_k$ , the spectral distribution  $\mu$  under question is characterized by the property of orthonormal polynomials  $\{Q_k\}$  defined recurrently by

$$Q_0(x) = 1, \quad Q_1(x) = x,$$

$$xQ_k(x) = Q_{k+1}(x) + \alpha_k Q_k(x) + \beta_k^2 Q_{k-1}(x), \quad k \geq 1. \quad (2-20)$$

If such a spectral distribution is unique, the spectral distribution  $\mu$  is determined by the identity

$$G_\mu(x) = \int_R \frac{\mu(dy)}{x-y} = \frac{1}{x - \alpha_0 - \frac{\beta_1^2}{x - \alpha_1 - \frac{\beta_2^2}{x - \alpha_2 - \frac{\beta_3^2}{x - \alpha_3 - \dots}}}} = \frac{Q_{d-1}^{(1)}(x)}{Q_d(x)} = \sum_{l=0}^{d-1} \frac{A_l}{x - x_l}, \quad (2-21)$$

where,  $x_l$  are the roots of polynomial  $Q_d(x)$ .  $G_\mu(z)$  is called the Stieltjes function (Stieltjes/Hilbert transform of spectral distribution  $\mu$ ) and polynomials  $\{Q_k^{(1)}\}$  are defined recurrently as

$$Q_0^{(1)}(x) = 1, \quad Q_1^{(1)}(x) = x - \alpha_1,$$



$$xQ_k^{(1)}(x) = Q_{k+1}^{(1)}(x) + \alpha_{k+1}Q_k^{(1)}(x) + \beta_{k+1}^2Q_{k-1}^{(1)}(x), \quad k \geq 1, \quad (2-22)$$

respectively. Then, from (2-21), one can see that the spectral distribution  $\mu$  is written as

$$\mu(x) = \sum_{l=0}^{d-1} A_l \delta(x - x_l). \quad (2-23)$$

The coefficients  $A_l$  appearing in (2-21) and (2-23) are calculated as

$$A_l = \lim_{x \rightarrow x_l} (x - x_l) G_\mu(x). \quad (2-24)$$

(for more details see Refs.[17, 18, 19, 20].)

### 3 Continuous-time quantum walk on an arbitrary graph

For a Given undirected graph  $\Gamma$  with  $n$  vertices and adjacency matrix  $A$ , one can define the Laplacian of  $\Gamma$  as  $L = A - D$ , where  $D$  is the diagonal matrix with  $D_{jj} = \deg(j)$ , the degree of vertex  $j$ . Classically, suppose that  $P(t)$  is a time-dependent probability distribution of a stochastic (particle) process on  $\Gamma$ . The classical evolution of the continuous-time walk is given by the Kolmogorov equation

$$\frac{dP(t)}{dt} = LP(t). \quad (3-25)$$

The solution to this equation, modulo some conditions, is  $P(t) = e^{tL}P(0)$ , which can be solved by diagonalizing the symmetric matrix  $L$ . This spectral approach requires full knowledge of the spectrum of  $L$ .

A quantum analogue of the classical walk, the so-called CTQW, uses the Schrödinger equation in place of the Kolmogorov equation, where  $L$  is chosen as the Hamiltonian of the walk. This is because we can view  $L$  as the generator matrix that describes an exponential distribution of waiting times at each vertex. Let  $|\phi(t)\rangle$  be a time-dependent amplitude of the quantum process on  $\Gamma$ . Then, the wave evolution of the quantum walk is governed by

$$i\hbar \frac{d}{dt} |\phi(t)\rangle = H |\phi(t)\rangle. \quad (3-26)$$

Assuming  $\hbar = 1$  for simplicity, the solution to (3-26) is given by  $|\phi(t)\rangle = e^{-iHt}|\phi(0)\rangle$  which, again, is solvable via spectral techniques. On  $d$ -regular graphs, we have  $D = \frac{1}{d}I$ , and since  $A$  and  $D$  commute, we get

$$e^{-itH} = e^{-it(A - \frac{1}{d}I)} = e^{it/d}e^{-itA}. \quad (3-27)$$

This introduces an irrelevant phase factor in the wave evolution. Hence we can consider  $H = A = A_1$ . Thus, we have

$$|\phi(t)\rangle = e^{-iAt}|\phi(0)\rangle. \quad (3-28)$$

In the case of distance regular graphs, according to (4-43) the adjacency matrices are polynomial functions of  $A$ , hence by using (2-16) and (2-17), the matrix elements  $\langle \phi_l | A^m | \phi_0 \rangle$  for  $m = 0, 1, \dots$  can be written as

$$\langle \phi_l | A^m | \phi_0 \rangle = \langle \phi_0 | P'_l(A) A^m | \phi_0 \rangle = \int_R x^m P'_l(x) \mu(dx). \quad (3-29)$$

By using (3-29), the probability amplitude of observing the walk at  $l$ -th stratum at time  $t$  can be evaluated as

$$q_l(t) \equiv \langle \phi_l | e^{-iAt} | \phi_0 \rangle = \int_R e^{-ixt} P'_l(x) \mu(dx) = \frac{1}{\sqrt{\omega_1 \dots \omega_l}} \int_R e^{-ixt} Q_l(x) \mu(dx). \quad (3-30)$$

In particular, the probability of observing the walk at starting site at time  $t$  is given by

$$q_0(t) = \langle \phi_0 | e^{-iAt} | \phi_0 \rangle = \int_R e^{-ixt} \mu(dx). \quad (3-31)$$

The conservation of probability  $\sum_{l=0} |\langle \phi_l | \phi_0(t) \rangle|^2 = 1$  follows immediately from (3-30) by using the completeness relation of orthogonal polynomials  $P_l(x)$ .

We notice that the formula (3-30) indicates a canonical isomorphism between the interacting Fock space of CTQW on distance regular graphs and the closed linear span of the orthogonal polynomials generated by recursion relations (4-42). This isomorphism was meant to be, a reformulation of CTQW (on distance regular graphs), which describes quantum states by polynomials (describing quantum state  $|\phi_k\rangle$  by  $P_k(x)$ ), and make a correspondence between

functions of operators ( $q$ -numbers) and functions of classical quantity ( $c$ -numbers), such as the correspondence between  $e^{-iAt}$  and  $e^{-ixt}$ . This isomorphism is similar to the isomorphism between Fock space of annihilation and creation operators  $a, a^\dagger$  with space of functions of coherent states' parameters in quantum optics, or the isomorphism between Hilbert space of momentum and position operators, and spaces of function defined on phase space in Wigner function formalism.

According to the result of Ref. [11], the walk has the same probability amplitudes at all sites belonging to the same stratum and so the evaluation of  $q_l(t)$  leads to the determination of the amplitudes at sites belonging to the  $l$ -th stratum  $V_l(o)$ . Then, by using (2-4) we have

$$q_l(t) = \langle \phi_l | e^{-iAt} | \phi_0 \rangle = \frac{1}{\sqrt{\kappa_l}} \sum_{\alpha \in V_l(o)} \langle \alpha | e^{-iAt} | o \rangle = \sqrt{\kappa_l} \langle \alpha | e^{-iAt} | o \rangle. \quad (3-32)$$

Therefore, the probability amplitude of observing the walk at the site  $\alpha \in V_l(o)$  at time  $t$  is given by

$$p_\alpha(t) \equiv \langle \alpha | e^{-iAt} | o \rangle = \frac{1}{\sqrt{\kappa_l}} q_l(t) \quad , \quad \text{for all } \alpha \in V_l(o). \quad (3-33)$$

### 3.1 Evaluation of probability amplitudes by using Laplace transform

In this section, we give a procedure for calculating the probability amplitudes of CTQWs on graphs by using the Laplace transformation. To do so, first we give the definition of the Laplace transform. The Laplace transform of a time-dependent function  $f(t)$ , denoted by  $\hat{f}(s) = Lf(t)$ , is defined as

$$\hat{f}(s) = \int_0^\infty e^{-st} f(t) dt. \quad (3-34)$$

The Laplace transform has the following basic properties :

Linearity :  $L\{af(t) + bg(t)\} = a\hat{f}(s) + b\hat{g}(s)$ ,

Derivative :  $Lf'(t) = s\hat{f}(s) - f(0)$ ,

Shifting :  $Le^{at}f(t) = \hat{f}(s - a)$ .

(for more information related to the Laplace transform see [32],[22] and [23]).

By taking the Laplace transform of the amplitudes  $q_l(t)$  in (3-30) and using the equation (2-23), one can obtain

$$\begin{aligned}\hat{q}_l(s) &= \frac{1}{\sqrt{\omega_1 \dots \omega_l}} \int_0^\infty e^{-st} \int_R e^{-ixt} Q_l(x) \mu(dx) dt = \frac{1}{\sqrt{\omega_1 \dots \omega_l}} \sum_i A_i Q_l(x_i) \int_0^\infty e^{-(s+ix_i)t} dt = \\ &= \frac{1}{\sqrt{\omega_1 \dots \omega_l}} \sum_i \frac{A_i Q_l(x_i)}{s + ix_i} = \frac{i}{\sqrt{\omega_1 \dots \omega_l}} \sum_i \frac{A_i Q_l(x_i)}{is - x_i}.\end{aligned}\quad (3-35)$$

Therefore, although it is not an easy work in the most cases, the probability amplitudes  $q_l(t)$  of the walk can be obtained by taking the inverse Laplace transform of (3-35), but we have no need to do so. Instead, we calculate only  $\hat{q}_0(s)$  as follows

$$\hat{q}_0(s) = \int_0^\infty e^{-st} \int_R e^{-ixt} \mu(dx) dt = i \sum_i \frac{A_i}{is - x_i} = iG_\mu(is). \quad (3-36)$$

and obtain the probability amplitude of observing the walk at starting site at time  $t$  as

$$q_0(t) = iL^{-1}(G_\mu(is)). \quad (3-37)$$

From the formulas (3-30) and (3-31), it can be easily seen that

$$q_l(t) = P'_l(i \frac{d}{dt}) q_0(t) = \frac{1}{\sqrt{\omega_1 \dots \omega_l}} Q_l(i \frac{d}{dt}) q_0(t). \quad (3-38)$$

In fact, we need only to know the probability amplitude of observing the walk at starting site at time  $t$  and the polynomials  $Q_l(x)$  which are obtained via the recursion relations (2-20). Then, by using the equations (3-37) and (3-38), the probability amplitudes  $q_l(t)$  can be evaluated.

It could be noticed that, in this approach we do not any need to take the inverse Stieltjes transform to obtain the spectral measure  $\mu$ ; Instead we take the inverse Laplace transform of the Stieltjes function  $G_\mu(is)$  which is more popular and convenient (there are many handbooks and tables of Laplace transforms [32],[22],[23] and computer programmings for this purpose) in comparison with the inverse Stieltjes transform. In the following section, we calculate the probability amplitudes for CTQW on some important QD graphs, i.e., distance-regular graphs and some non-QD type graphs, explicitly.

## 4 Examples

In this section we consider CTQW on some examples of graphs and calculate the corresponding probability amplitudes of the walk on them by employing the techniques introduced in the previous section.

### 4.1 Examples of distance-regular graphs

In this subsection first we consider some set of important QD graphs called distance-regular graphs. To do so, we recall the definitions and properties related to distance-regular graphs:

**Definition.** An undirected connected graph  $G = (V, E)$  is called distance-regular graph (DRG) with diameter  $d$  if it satisfies the following distance-regularity condition:

For all  $h, i, j \in \{0, 1, \dots, d\}$ , and  $\alpha, \beta$  with  $\partial(\alpha, \beta) = h$ , the number

$$p_{ij}^k = |\{\gamma \in V : \partial(\alpha, \beta) = i \text{ and } \partial(\gamma, \beta) = j\}| \quad (4-39)$$

is constant in that it depends only on  $h, i, j$  but does not depend on the choice of  $\alpha$  and  $\beta$ .

Then,  $p_{ij}^h := |V_i(\alpha) \cap V_j(\beta)|$  for all  $\alpha, \beta \in V$  with  $\partial(\alpha, \beta) = h$ . This number is called the intersection number. In a distance regular graph,  $p_{j1}^i = 0$  (for  $i \neq 0$ ,  $j$  is not  $\{i-1, i, i+1\}$ ).

The intersection numbers of the graph are defined as

$$a_i = p_{i1}^i, \quad b_i = p_{i+1,1}^i, \quad c_i = p_{i-1,1}^i \quad (4-40)$$

These intersection numbers and the valencies  $\kappa_i$  satisfy the following obvious conditions

$$\begin{aligned} a_i + b_i + c_i &= \kappa_i, \quad \kappa_{i-1}b_{i-1} = \kappa_i c_i, \quad i = 1, \dots, d, \\ \kappa_0 &= c_1 = 1, \quad b_0 = \kappa_1 = \kappa, \quad (c_0 = b_d = 0). \end{aligned} \quad (4-41)$$

Thus, all parameters of the graph can be obtained from the intersection array  $\{b_0, \dots, b_{d-1}; c_1, \dots, c_d\}$ .

It could be noticed that, for adjacency matrices of a distance regular graph, we have

$$A_1 A_i = b_{i-1} A_{i-1} + a_i A_i + c_{i+1} A_{i+1}, \quad \text{for } i = 1, 2, \dots, d-1,$$

$$A_1 A_d = b_{d-1} A_{d-1} + a_d A_d. \quad (4-42)$$

Using the recursion relations (4-42), one can show that  $A_i$  is a polynomial in  $A_1$  of degree  $i$ , i.e., we have

$$A_i = P_i(A_1), \quad i = 1, 2, \dots, d, \quad (4-43)$$

and conversely  $A_1^i$  can be written as a linear combination of  $I, A_1, \dots, A_d$  (for more details see for example [11]).

It should be noticed that, for distance-regular graphs, the unit vectors  $|\phi_i\rangle$  for  $i = 0, 1, \dots, d$  defined as in (2-4), satisfy the following three-term recursion relations

$$A|\phi_i\rangle = \beta_{i+1}|\phi_{i+1}\rangle + \alpha_i|\phi_i\rangle + \beta_i|\phi_{i-1}\rangle, \quad (4-44)$$

where, the coefficients  $\alpha_i$  and  $\beta_i$  are defined as

$$\alpha_k = \kappa - b_k - c_k, \quad \omega_k \equiv \beta_k^2 = b_{k-1}c_k, \quad k = 1, \dots, d, \quad (4-45)$$

i.e., in the basis of unit vectors  $\{|\phi_i\rangle, i = 0, 1, \dots, d\}$ , the adjacency matrix  $A$  is projected to the following symmetric tridiagonal form:

$$A = \begin{pmatrix} \alpha_0 & \beta_1 & 0 & \dots & \dots & 0 \\ \beta_1 & \alpha_1 & \beta_2 & 0 & \dots & 0 \\ 0 & \beta_2 & \alpha_3 & \beta_3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \beta_{d-1} & \alpha_{d-1} & \beta_d \\ 0 & \dots & 0 & 0 & \beta_d & \alpha_d \end{pmatrix}. \quad (4-46)$$

In the following, we consider CTQW on some examples of distance-regular graphs in details, where in the Appendix A, we give a table of important distance-regular graphs together with the corresponding probability amplitude  $q_0(t)$ .

#### 4.1.1 Complete graph $K_n$

The complete graph  $K_n$  is the simplest example of distance-regular graphs. This graph has  $n$  vertices with  $n(n-1)/2$  edges, the degree of each vertex is  $\kappa = n-1$  also the graph has diameter  $d = 1$ . The intersection array of the graph is  $\{b_0; c_1\} = \{n-1; 1\}$ . Then, the graph has only two strata  $V_0(\alpha) = \alpha$  and  $V_1(\alpha) = \{\beta : \beta \neq \alpha\}$  with QD parameters  $\{\alpha_1; \omega_1\} = \{n-2, n-1\}$ . By using (2-21), the Stieltjes function is calculated as

$$G_\mu(x) = \frac{x - n + 2}{x^2 - (n-2)x - n + 1}. \quad (4-47)$$

From (3-36) and (4-47), we obtain

$$\hat{q}_0(s) = \frac{s + i(n-2)}{s^2 + is(n-2) + n-1} = \frac{1}{n} \left\{ \frac{1}{s + i(n-1)} + \frac{n-1}{s-i} \right\}. \quad (4-48)$$

Therefore, by taking the inverse Laplace transform of (4-78), we obtain the probability amplitude of observing the walk at starting site at time  $t$  as follows

$$q_0(t) = L^{-1}(\hat{q}_0(s)) = \frac{1}{n} (e^{-i(n-1)t} + (n-1)e^{it}). \quad (4-49)$$

For calculating the probability amplitude  $q_1(t)$ , first recall that  $\kappa_1 = n-1$  and  $P'_1(x) = \frac{x}{\sqrt{n-1}}$ , then by using (3-38) we obtain

$$q_1(t) = \frac{i}{\sqrt{n-1}} \frac{d}{dt} q_0(t) = \frac{\sqrt{n-1}}{n} (e^{-i(n-1)t} - e^{it}). \quad (4-50)$$

#### 4.1.2 Strongly regular graphs

For strongly regular graphs we have three strata and two kinds of two-point resistances  $R_{\alpha\beta(1)}$  and  $R_{\alpha\beta(2)}$ . The QD parameters of the graph with parameters  $(v, \kappa, \lambda, \mu)$  are given by

$$\alpha_1 = \lambda, \quad \alpha_2 = \kappa - \mu; \quad \omega_1 = \kappa, \quad \omega_2 = \mu(\kappa - \lambda - 1). \quad (4-51)$$

Then, by using (2-21) and (3-36), one can obtain

$$\hat{q}_0(s) = \frac{s^2 + i(\kappa + \lambda - \mu)s - \kappa(\lambda - \mu) - \mu}{s^3 + i(\kappa + \lambda - \mu)s^2 + (\kappa(\mu - \lambda + 1) - \mu)s + i\kappa(\kappa - \mu)}. \quad (4-52)$$

Therefore, the probability amplitude  $q_0(t)$  can be obtained as follows

$$q_0(t) = A_1 e^{-i\kappa t} + A_2 e^{-\frac{i}{2}(\lambda-\mu+\sqrt{(\lambda-\mu)^2-4(\mu-\kappa)})t} + A_3 e^{-\frac{i}{2}(\lambda-\mu+\sqrt{(\lambda-\mu)^2-4(\mu-\kappa)})t}, \quad (4-53)$$

where,

$$\begin{aligned} A_1 &= \frac{\mu}{\kappa^2 - \kappa(\lambda - \mu) + (\mu - \kappa)}, \\ A_2 &= \frac{-\kappa\sqrt{(\lambda - \mu)^2 - 4(\mu - \kappa)} + \kappa(\lambda - \mu) + 2\kappa}{(\lambda - \mu - 2\kappa)\sqrt{(\lambda - \mu)^2 - 4(\mu - \kappa)} + (\lambda - \mu)^2 - 4(\mu - \kappa)}, \\ A_3 &= \frac{\kappa\sqrt{(\lambda - \mu)^2 - 4(\mu - \kappa)} + \kappa(\lambda - \mu) + 2\kappa}{(-\lambda + \mu + 2\kappa)\sqrt{(\lambda - \mu)^2 - 4(\mu - \kappa)} + (\lambda - \mu)^2 - 4(\mu - \kappa)}. \end{aligned} \quad (4-54)$$

In the remaining part of this example, we study CTQW on the following two well-known strongly regular graphs:

### A. Petersen graph

The Petersen graph [27] is a strongly regular graph with parameters  $(v, \kappa, \lambda, \mu) = (10, 3, 0, 1)$ , the intersection array  $\{b_0, b_1; c_1, c_2\} = \{3, 2; 1, 1\}$  and QD parameters  $\{\alpha_1, \alpha_2; \omega_1, \omega_2\} = \{0, 2; 3, 2\}$ . Then, by using (4-54), we obtain

$$A_1 = \frac{1}{10}, \quad A_2 = \frac{1}{2}, \quad A_3 = \frac{2}{5}. \quad (4-55)$$

By substituting (4-55) in (4-53), we obtain the probability amplitude of observing the walk at starting site at time  $t$  as follows

$$q_0(t) = \frac{1}{10}(5e^{-it} + 4e^{2it} + e^{-3it}). \quad (4-56)$$

Then the probability amplitudes  $q_1(t)$  and  $q_2(t)$  are easily calculated as

$$\begin{aligned} q_1(t) &= \frac{i}{\sqrt{3}} \frac{d}{dt} q_0(t) = \frac{1}{\sqrt{3}} \left( \frac{1}{2} e^{-it} - \frac{4}{5} e^{2it} + \frac{3}{10} e^{-3it} \right), \\ q_2(t) &= \frac{1}{\sqrt{6}} \left( -\frac{d^2}{dt^2} - 3 \right) q_0(t) = \frac{1}{\sqrt{6}} \left( -e^{-it} + \frac{2}{5} e^{2it} + \frac{2}{5} e^{-3it} \right). \end{aligned} \quad (4-57)$$

### B. Normal subgroup scheme

**Definition** The partition  $P = \{P_0, P_1, \dots, P_d\}$  of a finite group  $G$  is called a blueprint if



(i)  $P_0 = \{e\}$

(ii) for  $i=1,2,\dots,d$  if  $g \in P_i$  then  $g^{-1} \in P_i$

(iii) the set of relations  $R_i = \{(\alpha, \beta) \in G \otimes G | \alpha^{-1}\beta \in P_i\}$  on  $G$  form an association scheme[27].

The set of real conjugacy classes given in Appendix A of Ref. [11] is an example of blueprint on  $G$ . Also, one can show that in the regular representation, the class sums  $\bar{P}_i$  for  $i = 0, 1, \dots, d$  defined as

$$\bar{P}_i = \sum_{\gamma \in P_i} \gamma \in CG, \quad i = 0, 1, \dots, d, \quad (4-58)$$

are the adjacency matrices of a blueprint scheme.

In Ref.[11], it has been shown that, if  $H$  be a normal subgroup of  $G$ , the following blueprint classes

$$P_0 = \{e\}, \quad P_1 = G - \{H\}, \quad P_2 = H - \{e\}, \quad (4-59)$$

define a strongly regular graph with parameters  $(v, \kappa, \lambda, \mu) = (g, g - h, g - 2h, g - h)$  and the following intersection array

$$\{b_0, b_1; c_1, c_2\} = \{g - h, h - 1; 1, g - h\}, \quad (4-60)$$

where,  $g := |G|$  and  $h := |H|$ . It is interesting to note that in normal subgroup scheme, the intersections numbers and other parameters depend only on the cardinalities of the group and its normal subgroup. By using (4-45), the QD parameters are given by  $\{\alpha_1, \alpha_2; \omega_1, \omega_2\} = \{g - 2h, 0; g - h, (g - h)(h - 1)\}$ .

As an example, we consider the dihedral group  $G = D_{2m}$ , where its normal subgroup is  $H = Z_m$ . Therefore, the blueprint classes are given by

$$P_0 = \{e\}, \quad P_1 = \{b, ab, a^2b, \dots, a^{m-1}b\}, \quad P_2 = \{a, a^2, \dots, a^{(m-1)}\}, \quad (4-61)$$

which form a strongly regular graph with parameters  $(2m, m, 0, m)$  and the following intersection numbers and QD parameters

$$\{b_0, b_1; c_1, c_2\} = \{m, m - 1; 1, m\}; \quad \{\alpha_1, \alpha_2; \omega_1, \omega_2\} = \{0, 0; m, m(m - 1)\}. \quad (4-62)$$

Then, by using (4-54), we obtain

$$A_1 = \frac{1}{2m}, \quad A_2 = \frac{m-1}{m}, \quad A_3 = \frac{1}{2m}. \quad (4-63)$$

Now, by substituting (4-63) in (4-53), we obtain the probability amplitude of observing the walk at starting site at time  $t$  as follows

$$q_0(t) = \frac{1}{m}(m-1 + \cos mt). \quad (4-64)$$

The other probability amplitudes are calculated as

$$\begin{aligned} q_1(t) &= \frac{i}{\sqrt{m}} \frac{d}{dt} q_0(t) = -\frac{i}{\sqrt{m}} \sin mt, \\ q_2(t) &= \frac{1}{\sqrt{m}} \left( -\frac{d^2}{dt^2} - m\sqrt{m} \right) q_0(t) = (\sqrt{m} - 1) \cos mt - (m-1). \end{aligned} \quad (4-65)$$

#### 4.1.3 Cycle graph $C_{2m}$

The cycle graph or cycle with  $n$  vertices is denoted by  $C_n$  with  $\kappa = 2$ . We consider  $n = 2m$  (the case  $n = 2m + 1$  can be considered similarly). The intersection array is given by

$$\{b_0, \dots, b_{m-1}; c_1, \dots, c_m\} = \{2, 1, \dots, 1, 1; 1, \dots, 1, 2\} \quad (4-66)$$

Then, by using (4-45), the QD parameters are given by

$$\alpha_i = 0, \quad i = 0, 1, \dots, m; \quad \omega_1 = \omega_m = 2, \quad \omega_i = 1, \quad i = 2, \dots, m-1, \quad (4-67)$$

Therefore, by using (2-21) and (3-36), one can obtain

$$\hat{q}_0(s) = \frac{i}{n} \frac{T'_n(\frac{is}{2})}{T_n(\frac{is}{2})}. \quad (4-68)$$

Then, the probability amplitude  $q_0(t)$  is obtained as

$$q_0(t) = \frac{1}{n} \left( \cos 2t + \sum_{l=1, l \neq n}^{2n-1} e^{-2it \cos \frac{2l\pi}{2n}} \right). \quad (4-69)$$

From (3-38), one can calculate

$$q_1(t) = \frac{1}{\sqrt{2}} \frac{d}{dt}(q_0(t)) = -\frac{\sqrt{2}i}{n} (\sin 2t + i \sum_{l=1, l \neq n}^{2n-1} \cos \frac{2l\pi}{2n} e^{-2it \cos \frac{2l\pi}{2n}}). \quad (4-70)$$

The amplitudes  $q_l(t)$ , for  $l > 1$  can be calculated similarly, where the results thus obtained are in agreement with those of Ref.[25].

It could be noticed that, in the limit of the large  $n$ , the cycle graph tend to the infinite line graph  $Z$  and the Stieltjes function reads as

$$G_\mu(x) = \frac{1}{\sqrt{x^2 - 4}}. \quad (4-71)$$

Therefore, by using (3-36) we obtain  $q_0(t)$  as follows

$$q_0(t) = L^{-1}(iG_\mu(is)) = J_0(2t), \quad (4-72)$$

where, the  $J_0$  is Bessel function. From (3-38), we can calculate

$$\begin{aligned} q_1(t) &= \frac{1}{\sqrt{2}} \frac{d}{dt}(J_0(2t)) = -\sqrt{2}iJ_1(2t), \\ q_2(t) &= \frac{1}{\sqrt{2}} \left(-\frac{d^2}{dt^2} - 2\right)(J_0(2t)) = -\sqrt{2}J_2(2t). \end{aligned} \quad (4-73)$$

By using (4-87), one can deduce that

$$q_l(t) = \sqrt{2}(-i)^l J_l(2t), \quad (4-74)$$

where the results are in agreement with those of Ref.[26].

#### 4.1.4 Johnson graphs

Let  $n \geq 2$  and  $d \leq n/2$ . The Johnson graph  $J(n, d)$  has all  $d$ -element subsets of  $\{1, 2, \dots, n\}$  such that two  $d$ -element subsets are adjacent if their intersection has size  $d - 1$ . Two  $d$ -element subsets are then at distance  $i$  if and only if they have exactly  $d - i$  elements in common. The

Johnson graph  $J(n, d)$  has  $v = \frac{n!}{d!(n-d)!}$  vertices, diameter  $d$  and the valency  $\kappa = d(n-d)$ . Its intersection array is given by

$$b_i = (d-i)(n-d-i), \quad 0 \leq i \leq d-1; \quad c_i = i^2, \quad 1 \leq i \leq d. \quad (4-75)$$

Then, by using (4-45) the QD parameters are given by

$$\alpha_k = k(n-2k), \quad \omega_k = k^2(d-k+1)(n-d-k+1). \quad (4-76)$$

For  $d = 2$ , the Stieltjes function is calculated as

$$G_\mu(x) = \frac{x-n+2}{x^2 - (n-2)x - 2(n-2)}. \quad (4-77)$$

Then by using (3-36) and (4-47), we obtain

$$\hat{q}_0(s) = \frac{s+i(n-2)}{s^2 + is(n-2) - 2(n-2)} = \frac{1}{2} \left\{ \frac{1 - \sqrt{\frac{n-2}{n+6}}}{s + i\left(\frac{n-2 + \sqrt{(n-2)(n+6)}}{2}\right)} + \frac{1 + \sqrt{\frac{n-2}{n+6}}}{s + i\left(\frac{n-2 - \sqrt{(n-2)(n+6)}}{2}\right)} \right\}. \quad (4-78)$$

Then, the probability amplitude  $q_0(t)$  can be obtained as follows

$$q_0(t) = L^{-1}(iG_\mu(is)) = e^{-i\frac{n-2}{2}t} \left\{ \cos\left(\frac{\sqrt{(n-2)(n+6)}}{2}t\right) + i\sqrt{\frac{n-2}{n+6}} \sin\left(\frac{\sqrt{(n-2)(n+6)}}{2}t\right) \right\}. \quad (4-79)$$

## 4.2 Examples of non-QD type graphs

### 4.2.1 Tchebichef graphs

By choosing Tchebichef polynomials of the first kind (the second kind) with scaling factor  $1/2^m$  as orthogonal polynomials appearing in the recursion relations (2-20), i.e.,  $Q_n(x) = 2^{(m-1)n+1}T_n(x/2^m)$  ( $2^{(m-1)n}U_n(x/2^m)$ ), one can obtain a class of finite and infinite graphs of Tchebichef type, with QD parameters  $\omega_1 = 2^{2(m-1)+1}$ ,  $\omega_k = 2^{2(m-1)}$ ,  $k = 2, 3, \dots$ , and  $\alpha_k = 0$ , for  $k = 1, 2, 3, \dots$  ( $\alpha_k = 0$ ;  $\omega_k = 2^{2(m-1)}$ ,  $k = 1, 2, \dots$ ). Then, we obtain

$$\hat{q}_0(s) = \frac{i}{n} \frac{T'_n\left(\frac{is}{2^m}\right)}{T_n\left(\frac{is}{2^m}\right)} \left( \frac{i}{2^{m-1}} \frac{U_n\left(\frac{is}{2^m}\right)}{U_{n+1}\left(\frac{is}{2^m}\right)} \right). \quad (4-80)$$

Therefore, the probability amplitude  $q_0(t)$  can be obtained as follows

$$q_0(t) = \frac{1}{n} \sum_{l=0}^{n-1} e^{-i2^m t \cos \frac{(2l+1)\pi}{2n}} \quad (4-81)$$

for the first kind and

$$q_0(t) = \frac{2}{n+2} \sum_{l=0}^{n-1} \sin^2 \frac{l\pi}{n+2} e^{-i2^m t \cos \frac{l\pi}{n+2}} \quad (4-82)$$

for the second kind.

#### 4.2.2 Finite path graph $P_n$

For  $m = 1$  in (4-80) and Tchebishef polynomials of the second kind we obtain finite path graph  $P_n = \{0, 1, 2, \dots, n-1\}$ , where it is a  $n$ -vertex graph with  $n-1$  edges all on a single open path [11]. For this graph, the stratification depends on the choice of the starting site of walk.

If we choose the first vertex as the starting site of the walk, the QD parameters are given by  $\omega_i = 1, \quad \alpha_i = 0, \quad i = 1, \dots, n-1$ . Then by using (4-82) we have

$$q_0(t) = \frac{2}{n+2} \sum_{k=1}^{n+1} \sin^2\left(\frac{k\pi}{n+2}\right) e^{-it \cos\left(\frac{k\pi}{n+2}\right)}. \quad (4-83)$$

From (3-38) and the recursion relations  $P'_{l+1}(x) = xP'_l(x) - P'_{l-1}(x)$ , one can obtain the probability amplitude of observing the walk at  $l$ -th stratum at time  $t$  as follows

$$q_l(t) = \frac{2}{n+2} \sum_{k=1}^{n+1} \sin\left(\frac{k\pi}{n+2}\right) \sin\left(\frac{(l+1)k\pi}{n+2}\right) e^{-it \cos\left(\frac{k\pi}{n+2}\right)}, \quad l \geq 1. \quad (4-84)$$

where the results thus obtained are in agreement with those of Ref.[26].

In the limit of the large  $n$ , one can calculate the Stieltjes function as follows

$$G_\mu(x) = \frac{1}{x - \frac{1}{x - \frac{1}{x - \frac{1}{x - \dots}}}} = \frac{1}{x - G_\mu(x)}, \quad (4-85)$$

then we obtain the following closed form for the Stieltjes function

$$G_\mu(x) = \frac{x - \sqrt{x^2 - 4}}{2}. \quad (4-86)$$

Therefore, by using (3-36) we have

$$\hat{q}_0(s) = \frac{\sqrt{s^2 + 4} - s}{2} \quad (4-87)$$

and then the probability amplitude of observing the walk at starting site at time  $t$  is given by

$$q_0(t) = J_0(2t) + J_2(2t). \quad (4-88)$$

Now, by using (3-38), the probability amplitudes  $q_l(t)$  are obtained as follows

$$q_l(t) = i^l (J_l(2t) + J_{l+2}(2t)). \quad (4-89)$$

### 4.2.3 The graphs $G_n$

For  $m = \frac{3}{2}$  in (4-80) and Tchebishef polynomials of the second kind we obtain a sequence of graphs denoted by  $G_n$  (for more details see Ref.[30]). The number of vertices in  $G_n$  is  $2^{n+1} + 2^n - 2$ . In general,  $G_n$  consists of two balanced binary trees of depth  $n$  with the  $2^n$ ,  $n$ -th level vertices of the two trees pairwise identified. For the quantum walk on  $G_n$ , we assume that the starting site of the walk is the root of a tree and calculate the probability amplitude of the presence of the walk at the other vertices as a function of time. Clearly, the graph  $G_n$  has  $(2n + 1)$  strata, where the  $j$ -th stratum consists of  $2^j$  vertices for  $j = 1, 2, \dots, n + 1$  and  $2^{2n+1-j}$  for  $j = n + 1, \dots, 2n + 1$ . The QD parameters are  $\omega_i = 2$ ,  $\alpha_i = 0$ ,  $i = 1, \dots, 2n$ .

By using (4-82) we obtain

$$q_0(t) = \frac{2}{n+2} \sum_{k=1}^{n+1} \sin^2\left(\frac{k\pi}{n+2}\right) e^{-i2\sqrt{2}t \cos(\frac{k\pi}{n+2})}. \quad (4-90)$$

From (3-38) and the recursion relations  $P'_{l+1}(x) = xP'_l(x) - 2P'_{l-1}(x)$ , one can obtain the probability amplitude of observing the walk at  $l$ -th stratum at time  $t$  as follows

$$q_l(t) = \frac{2}{n+2} \sum_{k=1}^{n+1} \sin\left(\frac{k\pi}{n+2}\right) \sin\left(\frac{(l+1)k\pi}{n+2}\right) e^{-i2\sqrt{2}t \cos(\frac{k\pi}{n+2})}, \quad l \geq 1. \quad (4-91)$$

In the limit of the large  $n$ , one can calculate the Stieltjes function as follows

$$G_\mu(x) = \frac{1}{x - \frac{2}{x - \frac{2}{x - \frac{2}{x - \dots}}}} = \frac{1}{x - 2G_\mu(x)}, \quad (4-92)$$

then we obtain the following closed form for the Stieltjes function

$$G_\mu(x) = \frac{x - \sqrt{x^2 - 8}}{4}. \quad (4-93)$$

Therefore, by using (3-36) we have

$$\hat{q}_0(s) = \frac{\sqrt{s^2 + 8} - s}{4} \quad (4-94)$$

and then the probability amplitude of observing the walk at starting site at time  $t$  is given by

$$q_0(t) = J_0(2\sqrt{2}t) + J_2(2\sqrt{2}t). \quad (4-95)$$

Now, by using (3-38), the probability amplitudes  $q_l(t)$  are obtained as follows

$$q_l(t) = i^l (J_l(2\sqrt{2}t) + J_{l+2}(2\sqrt{2}t)). \quad (4-96)$$

#### 4.2.4 Finite path graph with the second vertex as starting site of the walk

Now, we study an example of non-QD type graphs such that as the authors have shown in Ref. [15], one can give the three term recursion to the graph by using the Krylov-subspace Lanczos algorithm applied to the chosen reference state and the adjacency matrix of the graph and calculate the Stieltjes function (for more details see [15]). For instance, we consider the finite path graph and choose the second vertex of the graph as the starting site of the walk, then the graph does not satisfy three term recursion relations, i.e., the adjacency matrix has not tridiagonal form.

In Ref. [15], it has been shown that the QD parameters for  $P_n$  are given by  $\alpha_i = 0$  for  $i = 0, 1, \dots, 2k - 1$  and

$$\omega_{2i} = \frac{i}{i+1}, \quad \omega_{2i-1} = \frac{i+1}{i}, \quad \omega_{2k-1} = \frac{1}{k}; \quad i = 1, \dots, k-1.$$

for even values of  $n$ , where for odd values of  $n$  we have

$$\omega_{2i} = \frac{i}{i+1}, \quad i = 1, \dots, k-1.$$

$$\omega_{2i-1} = \frac{i+1}{i}, \quad i = 1, \dots, k,$$

Substituting these QD parameters in (2-20) and (2-22) and using (2-21), the Stieltjes function is obtained as

$$G_\mu(x) = \frac{xU_{n-2}(x/2)}{U_n(x/2)} \quad (4-97)$$

where,  $U_n$ 's are Tchebichef polynomials of the second kind. Therefore, by using (3-36) we have

$$\hat{q}_0(s) = \frac{-sU_{n-2}(is/2)}{U_n(is/2)}. \quad (4-98)$$

Then, the probability amplitude of the walk at starting site (the second vertex) at time  $t$  is given by

$$q_0(t) = \frac{1}{n+1} \sum_{l=1}^n \sin^2\left(\frac{2l\pi}{n+1}\right) e^{-2it \cos l\pi/(n+1)}, \quad (4-99)$$

again one can calculate the other probability amplitudes by using the Eq.(3-38).

## 5 Conclusion

CTQW on graphs was investigated by using the techniques based on spectral analysis of the graph and inverse Laplace transformation of the Stieltjes function associated with the graph. It was shown that the probability amplitudes of observing the walk at a given site at time  $t$  can be evaluated only by calculating the inverse Laplace transformation of the function  $iG_\mu(is)$  (without any knowledge about the spectrum of the graph), where  $G_\mu(x)$  is the Stieltjes function associated with the graph.

## Appendix A

In this appendix, we give the Laplace transform of the probability amplitude of observing the walk at starting site at time  $t$ ,  $\hat{q}_0(s)$ , for some important distance-regular graphs with  $n \leq 70$ .



The graph with Ref.	Intersection array	$q_0(s)$	$q_0(t)$
Icosahedron[28]	{5, 2, 1; 1, 2, 5}	$\frac{-i(is^4 - 4s^2 + 5is - 10)}{s^4 + 4is^3 + 10s^2 + 20is + 25}$	$\frac{1}{12}(5e^{it} + e^{-5it} + 6 \cos \sqrt{5}t)$
L(Petersen)[28]	{4, 2, 1; 1, 1, 4}	$\frac{-i(is^3 - 3s^2 + 4is - 4)}{s^4 + 3is^3 + 8s^2 + 12is + 16}$	$\frac{1}{18}(4e^{it} + e^{-4it} + 10 \cos 2t)$
Pappus, 3-cover $K_{3,3}$ [28]	{3, 2, 2, 1; 1, 1, 2, 3}	$\frac{s^4 + 9s^2 + 6}{s(s^4 + 12s^2 + 27)}$	$\frac{1}{18}(\cos 3t + \cos \sqrt{3}t + 2)$
$IG(AG(2, 4) \setminus pc)$ [30]	{4, 3, 3, 1; 1, 1, 3, 4}	$\frac{s^4 + 16s^2 + 12}{s(s^4 + 20s^2 + 64)}$	$\frac{1}{16}(\cos 4t + 12 \cos 2t + 3)$
3-cover $K_{9,9}$ [29]	{9, 8, 6, 1; 1, 3, 8, 9}	$\frac{s^4 + 81s^2 + 216}{s(s^4 + 90s^2 + 729)}$	$\frac{1}{27}(\cos 9t + 18 \cos 3t + 8)$
Odd(4)[32]	{4, 2, 1; 1, 1, 4}	$\frac{i(s^4 + 3is^3 + 13s^2 + 15is + 20)}{is^5 - 3s^4 + 18is^3 - 30s^2 + 65is - 75}$	$\frac{1}{18}(4e^{it} + e^{-4it} + 10 \cos 2t)$
$SRG \setminus \text{spread}$ [34]	{9, 6, 1; 1, 2, 9}	$\frac{-i(is^3 - 8s^2 + 9is - 18)}{s^4 + 8is^3 + 18s^2 + 72is + 8}$	$\frac{1}{40}(9e^{it} + e^{-9it} + 30 \cos 3t)$
3-cover $K_{6,6}$ [29]	{6, 5, 4, 1; 1, 2, 5, 6}	$\frac{-i(is^3 - 16s^2 + 17is - 136)}{s^4 + 16is^3 + 34s^2 + 272is + 289}$	$\frac{1}{36}(2 \cos 6t + 24 \cos \sqrt{6}t + 10)$
Hadamard graph[29]	{12, 11, 6, 1; 1, 6, 11, 12}	$\frac{s^4 + 144s^2 + 792}{s(s^4 + 156s^2 + 1728)}$	$\frac{1}{24}(\cos 12t + 12 \cos 2\sqrt{5}t + 8)$
$IG(AG(2, 5) \setminus pc)$ [30]	{5, 4, 4, 1; 1, 1, 4, 5}	$\frac{s^4 + 25s^2 + 20}{s(s^4 + 30s^2 + 125)}$	$\frac{1}{25}(\cos 5t + 20 \cos \sqrt{5}t + 11)$
Hadamard graph[31]	{8, 7, 4, 1; 1, 4, 7, 8}	$\frac{s^4 + 64s^2 + 224}{s(s^4 + 72s^2 + 512)}$	$\frac{1}{32}(2 \cos 8t + 16 \cos 2\sqrt{2}t + 14)$
Desargues[28]	{3, 2, 2, 1, 1; 1, 1, 2, 2, 3}	$\frac{s(s^4 + 11s^2 + 22)}{s^6 + 14s^4 + 49s^2 + 36}$	$\frac{1}{10}(\cos 3t + 4 \cos 2t + 10 \cos t)$
Klein[28]	{7, 4, 1; 1, 2, 7}	$\frac{-i(is^3 - 6s^2 + 7is - 14)}{s^4 + 6is^3 + 14s^2 + 42is + 49}$	$\frac{1}{24}(7e^{it} + e^{-7it} + 16 \cos \sqrt{7}t)$
$H(3, 3)$ [28]	{6, 4, 2; 1, 2, 3}	$\frac{-i(is^3 - 6s^2 + 3is - 24)}{s(s^3 + 6is^2 + 9s + 54i)}$	$\frac{1}{27}(e^{-6it} + 8e^{3it} + 6e^{-3it} + 12)$
coxeter[28]	{3, 2, 2, 1; 1, 1, 1, 2}	$\frac{i(s^4 + 21s^3 + 5s^2 + 6is + 2)}{is^5 - 2s^4 + 8is^3 - 12s^2 + 11is - 6}$	$\frac{1}{28}(19e^{it} + 8e^{-2it} + 12 \cos \sqrt{2}t)$
Mathon(Cycl(13, 3))[35]	{13, 8, 1; 1, 4, 13}	$\frac{-i(is^3 - 12s^2 + 13is - 52)}{s^4 + 12is^3 + 26s^2 + 156is + 169}$	$\frac{1}{42}(13e^{it} + e^{-13it} + 28 \cos \sqrt{13}t)$
Taylor( $P(17)$ )[29]	{17, 8, 1; 1, 8, 17}	$\frac{-i(is^3 - 3s^2 + 4is - 4)}{s^4 + 3is^3 + 8s^2 + 12is + 16}$	$\frac{1}{36}(17e^{it} + e^{-17it} + 18 \cos \sqrt{17}t)$
Taylor( $SRG(25, 12)$ )[29]	{25, 12, 1; 1, 12, 25}	$\frac{-i(is^3 - 24s^2 + 25is - 300)}{s^4 + 24is^3 + 50s^2 + 600is + 625}$	$\frac{1}{52}(25e^{it} + e^{-25it} + 26 \cos 5t)$
Mathon(Cycl(16, 3))[35]	{16, 10, 1; 1, 5, 16}	$\frac{-i(is^3 - 15s^2 + 16is - 80)}{s^4 + 15is^3 + 32s^2 + 240is + 256}$	$\frac{1}{51}(16e^{it} + e^{-16it} + 34 \cos 4t)$
Mathon(Cycl(11, 5))[35]	{11, 8, 1; 1, 2, 11}	$\frac{-i(is^3 - 10s^2 + 11is - 22)}{s^4 + 10is^3 + 22s^2 + 110is + 121}$	$\frac{1}{60}(11e^{it} + e^{-11it} + 48 \cos \sqrt{11}t)$
Mathon(Cycl(19, 3))[35]	{19, 12, 1; 1, 6, 19}	$\frac{-i(is^3 - 18s^2 + 19is - 114)}{s^4 + 18is^3 + 38s^2 + 342is + 361}$	$\frac{1}{60}(19e^{it} + e^{-19it} + 40 \cos \sqrt{19}t)$
Taylor( $SRG(29, 14)$ )[29]	{29, 14, 1; 1, 14, 29}	$\frac{-i(is^3 - 28s^2 + 29is - 406)}{s^4 + 28is^3 + 58s^2 + 812is + 841}$	$\frac{1}{60}(29e^{it} + e^{-29it} + 30 \cos \sqrt{29}t)$
Taylor( $P(13)$ )[29]	{13, 6, 1; 1, 6, 13}	$\frac{-i(is^3 - 12s^2 + 13is - 78)}{s^4 + 12is^3 + 26s^2 + 156is + 169}$	$\frac{1}{28}(13e^{it} + e^{-13it} + 14 \cos \sqrt{13}t)$
$GQ(2, 4) \setminus \text{spread}$ [28]	{8, 6, 1; 1, 3, 8}	$\frac{-i(is^3 - 5s^2 + 22is - 8)}{s^4 + 5is^3 + 30s^2 + 40is + 64}$	$\frac{1}{27}(8e^{it} + e^{-8it} + 12e^{-2it} + 6e^{4it})$
Doro	{12, 10, 3; 1, 3, 8}	$\frac{-i(is^3 - 11s^2 + 20is - 120)}{s(s^3 + 11is^2 + 32s + 240i)}$	$\frac{1}{68}(e^{-12it} + 17e^{-4it} + 16e^{5it} + 34)$
Locally Petersen	{10, 6, 4; 1, 2, 5}	$\frac{-i(is^3 - 12s^2 - 15is - 60)}{s(s^3 + 12is^2 - 5s + 150i)}$	$\frac{1}{65}(e^{-10it} + 13e^{-5it} + 25e^{3it} + 26)$
Taylor( $GQ(2, 2)$ )[29]	{15, 8, 1; 1, 8, 15}	$\frac{is^3 - 12s^2 + 43is - 90}{s^4 + 12is^3 + 58s^2 + 180is + 225}$	$\frac{1}{32}(15e^{it} + 6e^{5it} + 10e^{-3it} + e^{-15it})$
Taylor( $T(6)$ )[29]	{15, 6, 1; 1, 6, 15}	$\frac{-i(is^3 - 16s^2 - 13is - 120)}{s^4 + 16is^3 + 2s^2 + 240is + 225}$	$\frac{1}{32}(15e^{it} + 10e^{3it} + 6e^{-5it} + e^{-15it})$
Gosset, Tayl(Schläfli)[29]	{27, 10, 1; 1, 10, 27}	$\frac{-i(is^3 - 32s^2 - 129is - 432)}{s^4 + 32is^3 - 102s^2 + 864is + 729}$	$\frac{1}{56}(27e^{it} + e^{-27it} + 7e^{-9it} + 21e^{3it})$
Taylor(Co-Schläfli)[29]	{27, 16, 1; 1, 16, 27}	$\frac{-i(is^3 - 20s^2 + 183is - 270)}{s^4 + 20is^3 + 210s^2 + 540is + 729}$	$\frac{1}{56}(27e^{it} + e^{-27it} + 7e^{9it} + 21e^{-3it})$
$GH(2, 2)$ [29]	{6, 4, 4; 1, 1, 3}	$\frac{-i(is^3 - 5s^2 + 9is - 21)}{s^4 + 5is^3 + 15s^2 + 45is + 54}$	$\frac{1}{63}(27e^{it} + e^{-6it} + 14e^{3it} + 21e^{-3it})$
$H(3, 4)$ , Doob[29]	{9, 6, 3; 1, 2, 3}	$\frac{-i(is^3 - 12s^2 - 23is - 42)}{s^4 + 12is^3 - 14s^2 + 132is - 135}$	$\frac{1}{64}(27e^{-it} + 27e^{3it} + 9e^{-5it} + e^{-9it})$
Wells[30]	{5, 4, 1, 1; 1, 1, 4, 5}	$\frac{i(s^4 + 3is^3 + 13s^2 + 15is + 20)}{is^5 - 3s^4 + 18is^3 - 30s^2 + 65is - 75}$	$\frac{1}{32}(10e^{-it} + e^{-5it} + 5e^{3it} + 16 \cos \sqrt{5}t)$
$GH(2, 1)$ [28]	{4, 2, 2; 1, 1, 2}	$\frac{-i(is^3 - 4s^2 + is - 6)}{s^4 + 4is^3 + 5s^2 + 18is + 8}$	$\frac{1}{21}(e^{-4it} + 8e^{2it} + 12(e^{-it} + \cos \sqrt{2}t))$
$GH(3, 1)$ [36]	{6, 3, 3; 1, 1, 2}	$\frac{-i(is^3 - 8s^2 - 11is - 8)}{s^4 + 8is^3 - 5s^2 + 44is - 12}$	$\frac{1}{52}(e^{-6it} + 27e^{2it} + 24e^{-2it} + 24 \cos \sqrt{3}t)$
Dodecahedron[28]	{3, 2, 1, 1, 1; 1, 1, 1, 2, 3}	$\frac{-i(is^5 - 2s^4 + 7is^3 - 19s^2 + 10is - 6)}{s(s^5 + 2is^4 + 10s^3 + 16is^2 + 25s + 30i)}$	$\frac{1}{20}(5e^{-it} + 4e^{2it} + e^{-3it} + 6 \cos \sqrt{5}t + 4)$
Perkel[37]	{6, 5, 2; 1, 1, 3}	$\frac{-i(is^3 - 6s^2 + 2is - 15)}{s^4 + 8s^2 + 64is^3 + 51is - 18}$	$\frac{1}{57}(e^{-6it} + 20e^{3it} + 36e^{-3it/2} + 36 \cos \sqrt{5}/2t)$
$GO(2, 1)$ [30]	{4, 2, 2, 2; 1, 1, 1, 2}	$\frac{i(s^4 + 5is^3 - s^2 + 13is - 2)}{is^5 - 5s^4 + 3is^3 - 29s^2 + 21is - 24}$	$\frac{1}{45}(9e^{it} + 10e^{-it} + 16e^{2it} + 9e^{-3it} + e^{-4it})$
3-cover $GQ(2, 2)$ [30]	{6, 4, 2, 1; 1, 1, 4, 6}	$\frac{i(s^4 + 5is^3 + 11s^2 + 33is + 6)}{is^5 - 5s^4 + 17is^3 - 57s^2 + 72is - 108}$	$\frac{1}{45}(9e^{-it} + 18e^{2it} + 5e^{3it} + 12e^{-3it} + e^{-6it})$
$J(8, 4)$ [29]	{16, 9, 4, 1; 1, 4, 9, 16}	$\frac{i(s^4 + 20is^3 - 44s^2 + 368is - 192)}{is^5 - 20s^4 - 28is^3 - 592s^2 - 128is - 2048}$	$\frac{1}{70}(e^{-16it} + 7e^{-8it} + 28e^{2it} + 20e^{-2it} + 14e^{4it})$

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